



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 09:51 AM UTC

PDB ID : 6DJP / pdb_00006djp
EMDB ID : EMD-7939
Title : Integrin alpha-v beta-8 in complex with the Fabs 8B8 and 68
Authors : Cormier, A.; Campbell, M.G.; Nishimura, S.L.; Cheng, Y.
Deposited on : 2018-05-25
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

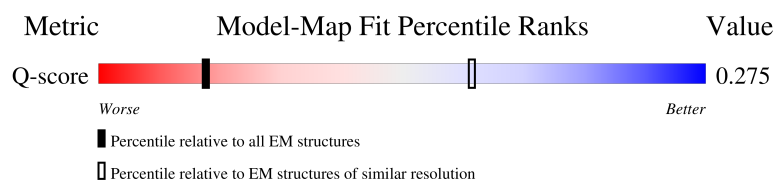
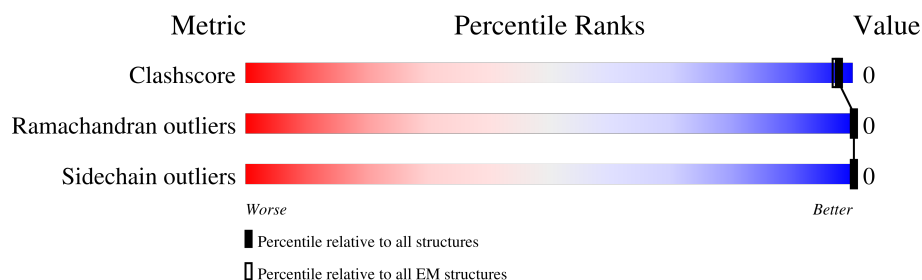
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	965	13% 58% 39%
2	B	639	6% 52% 45%
3	C	213	7% 53% 45%
4	D	213	8% 47% 50%

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Mol	Chain	Length	Quality of chain
5	E	212	
6	F	214	
7	G	2	
7	H	2	
7	J	2	
7	K	2	
7	L	2	
7	M	2	
8	I	6	
9	N	3	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7307 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-v.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	593	Total	C	N	O	0	0
			2979	1783	598	598		

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	353	Total	C	N	O	0	0
			1791	1075	358	358		

- Molecule 3 is a protein called 8B8 heavy chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	117	Total	C	N	O	0	0
			585	351	117	117		

- Molecule 4 is a protein called 8B8 light chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	107	Total	C	N	O	0	0
			536	322	107	107		

- Molecule 5 is a protein called 68 heavy chain Fab.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	115	Total	C	N	O	0	0
			569	339	115	115		

- Molecule 6 is a protein called 68 light chain Fab.

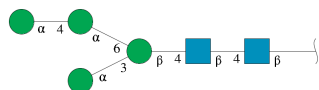
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	108	Total	C	N	O	0	0
			540	324	108	108		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



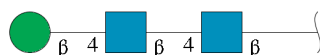
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	H	2	Total	C	N	O	0	0
			28	16	2	10		
7	J	2	Total	C	N	O	0	0
			28	16	2	10		
7	K	2	Total	C	N	O	0	0
			28	16	2	10		
7	L	2	Total	C	N	O	0	0
			28	16	2	10		
7	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

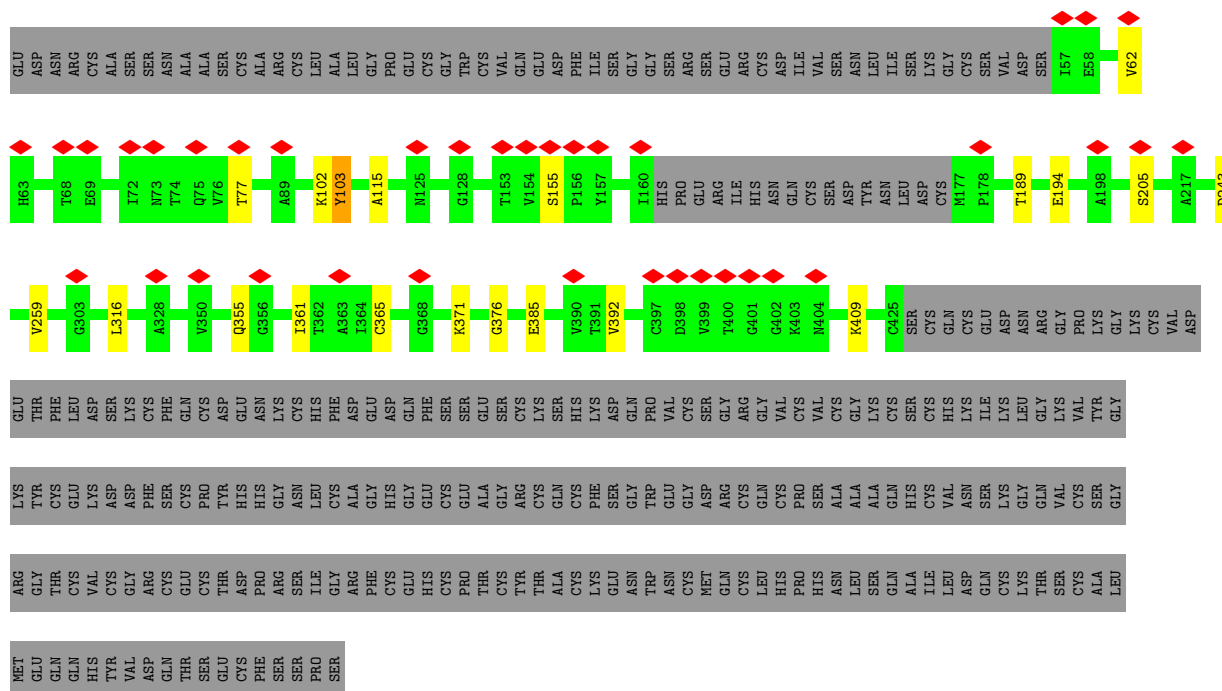


Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	3	Total	C	N	O	0	0
			39	22	2	15		

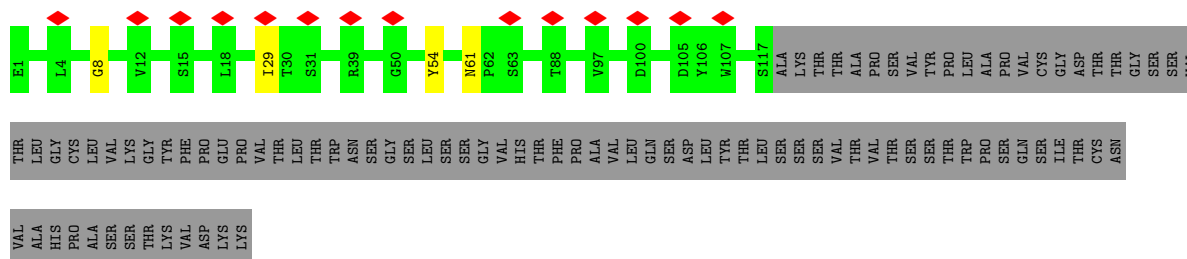
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



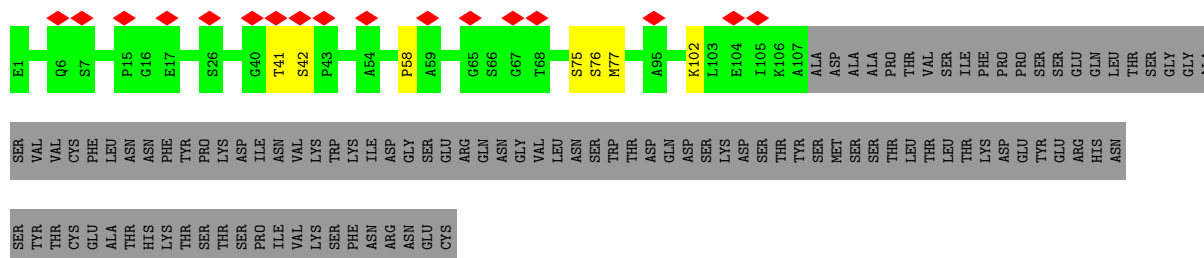
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	A	1	14	8	1	5	0
10	B	1	14	8	1	5	0



• Molecule 3: 8B8 heavy chain Fab



• Molecule 4: 8B8 light chain Fab



• Molecule 5: 68 heavy chain Fab



NAG1
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 8: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.069	Depositor
Minimum map value	-0.594	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.67, 1.67, 1.67	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	0/3006	1.50	55/4194 (1.3%)
2	B	0.77	1/1806 (0.1%)	1.52	24/2524 (1.0%)
3	C	0.78	0/588	1.47	6/820 (0.7%)
4	D	0.80	0/540	1.49	8/753 (1.1%)
5	E	0.81	0/571	1.38	5/793 (0.6%)
6	F	0.73	0/544	1.45	3/758 (0.4%)
All	All	0.77	1/7055 (0.0%)	1.49	101/9842 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	376	GLY	C-N	-6.13	1.24	1.33

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	61	ARG	N-CA-C	-9.30	102.74	114.56
1	A	400	MET	CA-C-N	8.95	126.19	119.66
1	A	400	MET	C-N-CA	8.95	126.19	119.66
6	F	32	TYR	N-CA-C	8.78	121.42	108.60
1	A	297	ALA	CA-C-N	8.62	128.35	119.56
1	A	297	ALA	C-N-CA	8.62	128.35	119.56
1	A	40	ALA	CA-C-N	8.60	128.33	119.56
1	A	40	ALA	C-N-CA	8.60	128.33	119.56
1	A	180	GLN	N-CA-C	-8.02	102.61	111.36
2	B	77	THR	N-CA-C	7.80	127.05	109.81
1	A	367	GLU	N-CA-C	-7.63	99.17	110.23
4	D	41	THR	N-CA-C	7.31	117.66	108.45
1	A	173	GLY	CA-C-N	7.25	126.96	119.56
1	A	173	GLY	C-N-CA	7.25	126.96	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	THR	N-CA-C	7.24	120.08	109.07
2	B	62	VAL	N-CA-C	7.17	118.96	109.21
2	B	103	TYR	CA-C-N	7.00	126.99	119.78
2	B	103	TYR	C-N-CA	7.00	126.99	119.78
2	B	385	GLU	CA-C-N	-6.98	113.37	122.37
2	B	385	GLU	C-N-CA	-6.98	113.37	122.37
1	A	296	GLY	CA-C-N	6.93	130.48	122.85
1	A	296	GLY	C-N-CA	6.93	130.48	122.85
4	D	77	MET	N-CA-C	6.79	119.59	110.35
2	B	371	LYS	CA-C-N	6.78	128.23	120.98
2	B	371	LYS	C-N-CA	6.78	128.23	120.98
2	B	243	ASP	N-CA-C	-6.75	105.67	114.04
1	A	196	ASP	CA-C-N	6.60	126.29	119.56
1	A	196	ASP	C-N-CA	6.60	126.29	119.56
1	A	466	THR	N-CA-C	6.59	116.76	108.45
1	A	401	PRO	CA-C-N	6.58	127.10	119.47
1	A	401	PRO	C-N-CA	6.58	127.10	119.47
1	A	544	ASP	CA-C-N	6.58	129.99	120.38
1	A	544	ASP	C-N-CA	6.58	129.99	120.38
5	E	52	LEU	CA-C-N	6.51	126.21	119.56
5	E	52	LEU	C-N-CA	6.51	126.21	119.56
3	C	29	ILE	N-CA-C	6.48	118.39	112.43
2	B	259	VAL	CA-C-N	6.35	126.27	119.85
2	B	259	VAL	C-N-CA	6.35	126.27	119.85
4	D	42	SER	CA-C-N	6.33	126.79	120.52
4	D	42	SER	C-N-CA	6.33	126.79	120.52
2	B	194	GLU	N-CA-C	-6.31	103.93	111.69
1	A	84	ASP	CA-C-N	6.30	126.25	119.76
1	A	84	ASP	C-N-CA	6.30	126.25	119.76
1	A	13	GLY	CA-C-N	6.26	126.21	119.76
1	A	13	GLY	C-N-CA	6.26	126.21	119.76
1	A	243	VAL	CA-C-N	6.23	126.70	119.47
1	A	243	VAL	C-N-CA	6.23	126.70	119.47
1	A	7	SER	CA-C-N	6.23	126.20	120.03
1	A	7	SER	C-N-CA	6.23	126.20	120.03
2	B	409	LYS	CA-C-N	6.20	125.95	119.76
2	B	409	LYS	C-N-CA	6.20	125.95	119.76
2	B	365	CYS	CA-C-N	6.16	125.85	119.56
2	B	365	CYS	C-N-CA	6.16	125.85	119.56
1	A	155	CYS	N-CA-C	6.15	118.77	111.33
5	E	97	ALA	N-CA-C	6.08	118.32	109.07
2	B	355	GLN	N-CA-C	6.07	118.67	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	LEU	CA-C-N	5.93	126.35	119.47
1	A	463	LEU	C-N-CA	5.93	126.35	119.47
1	A	368	ASP	N-CA-C	-5.93	103.97	110.91
3	C	54	TYR	N-CA-C	-5.92	104.90	111.71
1	A	575	GLN	CA-C-N	5.89	125.80	119.85
1	A	575	GLN	C-N-CA	5.89	125.80	119.85
3	C	8	GLY	CA-C-N	5.81	125.78	120.03
3	C	8	GLY	C-N-CA	5.81	125.78	120.03
1	A	514	LEU	N-CA-C	5.80	117.61	111.28
1	A	361	ALA	N-CA-C	5.80	118.22	109.23
4	D	42	SER	N-CA-C	5.79	122.61	109.81
1	A	339	ARG	CA-C-N	5.79	128.31	120.38
1	A	339	ARG	C-N-CA	5.79	128.31	120.38
1	A	29	SER	N-CA-C	-5.62	106.25	113.23
2	B	361	ILE	N-CA-C	5.58	115.57	107.88
1	A	205	ASN	N-CA-C	5.56	118.53	111.69
6	F	31	ASN	N-CA-C	5.50	119.48	112.12
1	A	27	VAL	CA-C-N	5.42	125.63	120.31
1	A	27	VAL	C-N-CA	5.42	125.63	120.31
1	A	570	ASP	CA-C-N	5.36	127.73	120.38
1	A	570	ASP	C-N-CA	5.36	127.73	120.38
4	D	102	LYS	N-CA-C	5.35	117.53	109.23
1	A	487	LEU	CA-C-N	5.33	125.31	120.03
1	A	487	LEU	C-N-CA	5.33	125.31	120.03
1	A	582	THR	CA-C-N	5.32	125.22	119.85
1	A	582	THR	C-N-CA	5.32	125.22	119.85
1	A	362	ALA	CA-C-N	5.29	124.95	119.56
1	A	362	ALA	C-N-CA	5.29	124.95	119.56
4	D	58	PRO	CA-C-N	5.27	128.07	120.38
4	D	58	PRO	C-N-CA	5.27	128.07	120.38
2	B	189	THR	N-CA-C	5.20	116.88	109.14
1	A	548	PHE	CA-C-N	5.17	128.86	120.60
1	A	548	PHE	C-N-CA	5.17	128.86	120.60
3	C	61	ASN	CA-C-N	5.14	126.27	119.84
3	C	61	ASN	C-N-CA	5.14	126.27	119.84
2	B	392	VAL	N-CA-C	5.14	116.06	108.45
2	B	155	SER	CA-C-N	5.07	124.73	119.56
2	B	155	SER	C-N-CA	5.07	124.73	119.56
5	E	40	ARG	CA-C-N	5.05	126.16	119.84
5	E	40	ARG	C-N-CA	5.05	126.16	119.84
1	A	518	SER	CA-C-N	5.04	124.70	119.56
1	A	518	SER	C-N-CA	5.04	124.70	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	GLY	N-CA-C	-5.04	103.65	112.77
2	B	316	LEU	CA-C-N	5.01	124.94	119.78
2	B	316	LEU	C-N-CA	5.01	124.94	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2979	0	1550	1	0
2	B	1791	0	884	2	0
3	C	585	0	267	0	0
4	D	536	0	280	1	0
5	E	569	0	283	0	0
6	F	540	0	262	1	0
7	G	28	0	25	0	0
7	H	28	0	25	0	0
7	J	28	0	25	0	0
7	K	28	0	25	0	0
7	L	28	0	25	0	0
7	M	28	0	25	0	0
8	I	72	0	57	0	0
9	N	39	0	33	0	0
10	A	14	0	13	0	0
10	B	14	0	13	0	0
All	All	7307	0	3792	5	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:SER:O	4:D:76:SER:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:O	1:A:64:THR:C	2.56	0.49
2:B:102:LYS:O	2:B:103:TYR:C	2.60	0.45
6:F:7:SER:N	6:F:8:PRO:CD	2.80	0.44
2:B:115:ALA:N	2:B:205:SER:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	591/965 (61%)	570 (96%)	21 (4%)	0	100	100
2	B	349/639 (55%)	334 (96%)	15 (4%)	0	100	100
3	C	115/213 (54%)	104 (90%)	11 (10%)	0	100	100
4	D	105/213 (49%)	98 (93%)	7 (7%)	0	100	100
5	E	113/212 (53%)	110 (97%)	3 (3%)	0	100	100
6	F	106/214 (50%)	99 (93%)	7 (7%)	0	100	100
All	All	1379/2456 (56%)	1315 (95%)	64 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	33/819 (4%)	33 (100%)	0	100	100
2	B	22/561 (4%)	22 (100%)	0	100	100
3	C	4/192 (2%)	4 (100%)	0	100	100
4	D	5/185 (3%)	5 (100%)	0	100	100
5	E	3/178 (2%)	3 (100%)	0	100	100
6	F	5/190 (3%)	5 (100%)	0	100	100
All	All	72/2125 (3%)	72 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

21 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	G	1	7,1	14,14,15	0.75	0	17,19,21	1.34	3 (17%)
7	NAG	G	2	7	14,14,15	1.02	1 (7%)	17,19,21	1.72	5 (29%)
7	NAG	H	1	7,1	14,14,15	0.89	0	17,19,21	1.00	1 (5%)
7	NAG	H	2	7	14,14,15	0.79	0	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	I	1	8,1	14,14,15	0.74	0	17,19,21	1.27	2 (11%)
8	NAG	I	2	8	14,14,15	0.87	1 (7%)	17,19,21	1.30	2 (11%)
8	BMA	I	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.94	1 (6%)
8	MAN	I	4	8	11,11,12	1.83	3 (27%)	15,15,17	1.11	1 (6%)
8	MAN	I	5	8	11,11,12	1.79	2 (18%)	15,15,17	1.09	2 (13%)
8	MAN	I	6	8	11,11,12	1.79	2 (18%)	15,15,17	1.03	2 (13%)
7	NAG	J	1	7,1	14,14,15	0.81	0	17,19,21	1.28	2 (11%)
7	NAG	J	2	7	14,14,15	0.90	1 (7%)	17,19,21	1.02	1 (5%)
7	NAG	K	1	2,7	14,14,15	0.79	0	17,19,21	1.11	2 (11%)
7	NAG	K	2	7	14,14,15	0.76	0	17,19,21	1.13	1 (5%)
7	NAG	L	1	2,7	14,14,15	0.86	1 (7%)	17,19,21	1.27	3 (17%)
7	NAG	L	2	7	14,14,15	0.79	0	17,19,21	0.96	1 (5%)
7	NAG	M	1	2,7	14,14,15	0.62	0	17,19,21	0.98	1 (5%)
7	NAG	M	2	7	14,14,15	0.79	0	17,19,21	1.02	1 (5%)
9	NAG	N	1	2,9	14,14,15	0.86	0	17,19,21	1.84	4 (23%)
9	NAG	N	2	9	14,14,15	0.91	1 (7%)	17,19,21	1.24	1 (5%)
9	BMA	N	3	9	11,11,12	1.80	2 (18%)	15,15,17	0.98	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1
7	NAG	H	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
8	NAG	I	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	2/2/19/22	0/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	1/2/19/22	0/1/1/1
8	MAN	I	6	8	-	1/2/19/22	0/1/1/1
7	NAG	J	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	NAG	L	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	1/6/23/26	0/1/1/1
7	NAG	M	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
9	NAG	N	1	2,9	-	4/6/23/26	0/1/1/1
9	NAG	N	2	9	-	1/6/23/26	0/1/1/1
9	BMA	N	3	9	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	5	MAN	O2-C2	-4.21	1.34	1.43
8	I	6	MAN	O2-C2	-4.17	1.34	1.43
8	I	4	MAN	O2-C2	-4.12	1.34	1.43
9	N	3	BMA	O2-C2	-4.12	1.34	1.43
8	I	3	BMA	O2-C2	-4.08	1.34	1.43
8	I	4	MAN	C4-C5	2.33	1.58	1.53
9	N	2	NAG	C3-C2	-2.29	1.47	1.52
9	N	3	BMA	C2-C3	-2.22	1.49	1.52
8	I	4	MAN	C2-C3	-2.18	1.49	1.52
8	I	6	MAN	C2-C3	-2.18	1.49	1.52
8	I	5	MAN	C2-C3	-2.17	1.49	1.52
8	I	3	BMA	C2-C3	-2.15	1.49	1.52
7	G	2	NAG	C3-C2	-2.13	1.48	1.52
7	J	2	NAG	C1-C2	2.08	1.55	1.52
8	I	2	NAG	C3-C2	-2.07	1.48	1.52
7	L	1	NAG	C3-C2	-2.04	1.48	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	1	NAG	O4-C4-C3	-3.92	101.14	110.38
9	N	2	NAG	C4-C3-C2	-3.58	105.77	111.02
7	G	2	NAG	C4-C3-C2	-3.49	105.90	111.02
7	H	2	NAG	C4-C3-C2	-3.34	106.12	111.02
7	K	2	NAG	C4-C3-C2	-3.28	106.22	111.02
7	G	1	NAG	O4-C4-C3	-3.22	102.78	110.38
9	N	1	NAG	O5-C1-C2	-3.21	106.33	111.29
7	G	2	NAG	O3-C3-C4	3.18	117.88	110.38
7	G	2	NAG	O4-C4-C3	3.04	117.55	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1	NAG	O4-C4-C3	-3.00	103.30	110.38
7	J	2	NAG	C4-C3-C2	-2.95	106.70	111.02
7	M	2	NAG	C4-C3-C2	-2.93	106.73	111.02
7	K	1	NAG	O4-C4-C3	-2.84	103.67	110.38
8	I	2	NAG	O5-C5-C6	-2.82	102.17	107.66
7	J	1	NAG	O4-C4-C3	-2.77	103.84	110.38
8	I	1	NAG	C3-C4-C5	-2.75	105.25	110.23
9	N	1	NAG	C3-C4-C5	-2.75	105.25	110.23
9	N	1	NAG	C1-O5-C5	2.66	115.75	112.19
7	L	2	NAG	C4-C3-C2	-2.66	107.12	111.02
7	L	1	NAG	O5-C5-C6	-2.48	102.84	107.66
7	M	1	NAG	C1-C2-N2	-2.43	106.61	110.43
8	I	5	MAN	C2-C3-C4	-2.37	106.69	110.86
7	G	1	NAG	O5-C5-C6	-2.34	103.10	107.66
8	I	3	BMA	C2-C3-C4	-2.29	106.83	110.86
8	I	6	MAN	C2-C3-C4	-2.24	106.92	110.86
7	G	2	NAG	C3-C4-C5	-2.23	106.19	110.23
7	G	2	NAG	O5-C1-C2	-2.22	107.86	111.29
7	H	1	NAG	C3-C4-C5	-2.19	106.27	110.23
8	I	1	NAG	O4-C4-C3	-2.18	105.23	110.38
7	L	1	NAG	C3-C4-C5	-2.18	106.29	110.23
8	I	5	MAN	C1-C2-C3	2.15	112.78	109.64
7	G	1	NAG	O4-C4-C5	-2.15	104.03	109.32
8	I	2	NAG	O4-C4-C3	-2.14	105.33	110.38
9	N	3	BMA	C2-C3-C4	-2.14	107.10	110.86
8	I	4	MAN	C3-C4-C5	-2.11	106.40	110.23
7	J	1	NAG	O5-C5-C6	-2.11	103.55	107.66
8	I	6	MAN	C1-C2-C3	2.09	112.69	109.64
7	K	1	NAG	C3-C4-C5	-2.03	106.55	110.23

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	2	NAG	O5-C5-C6-O6
7	M	2	NAG	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6

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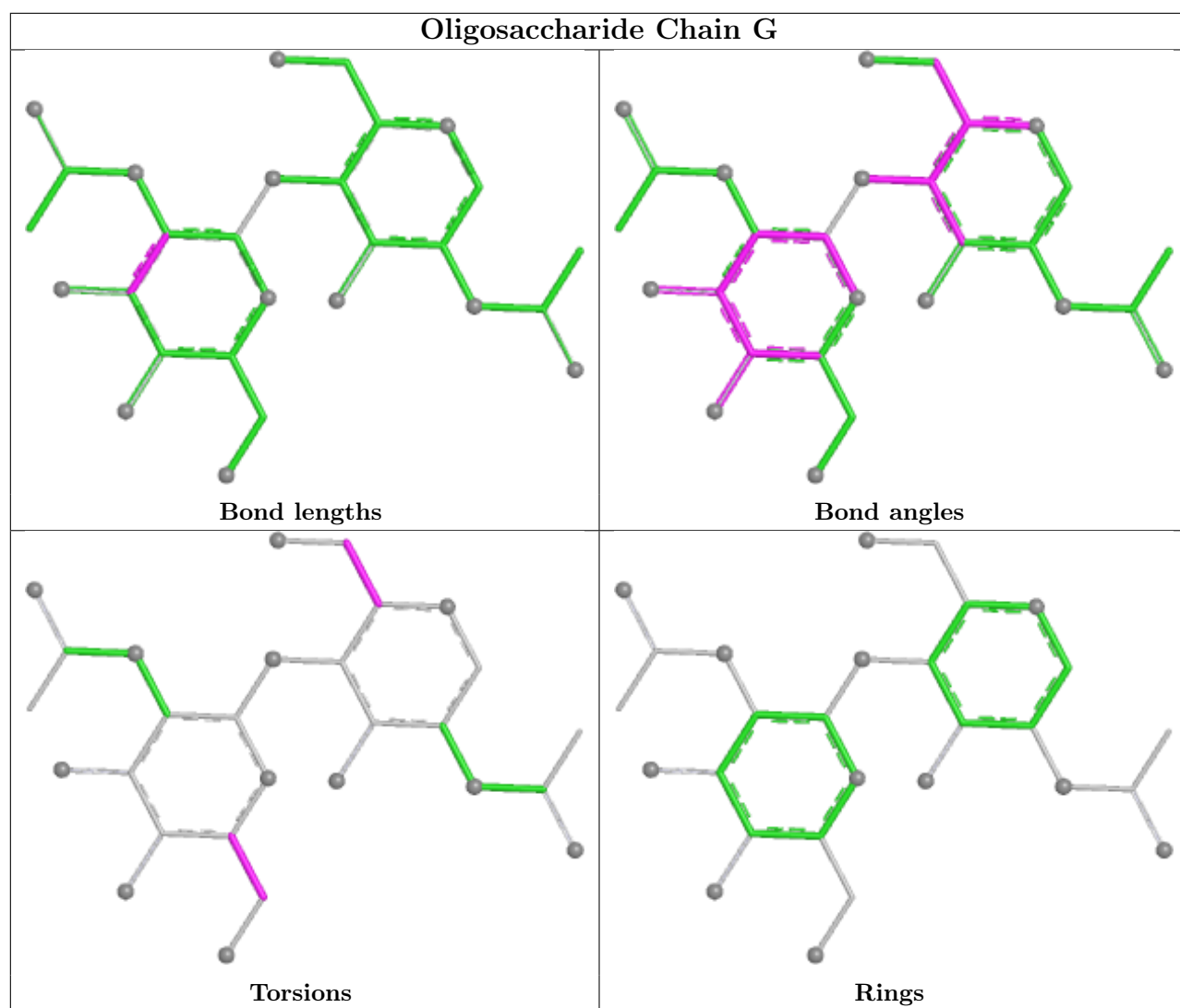
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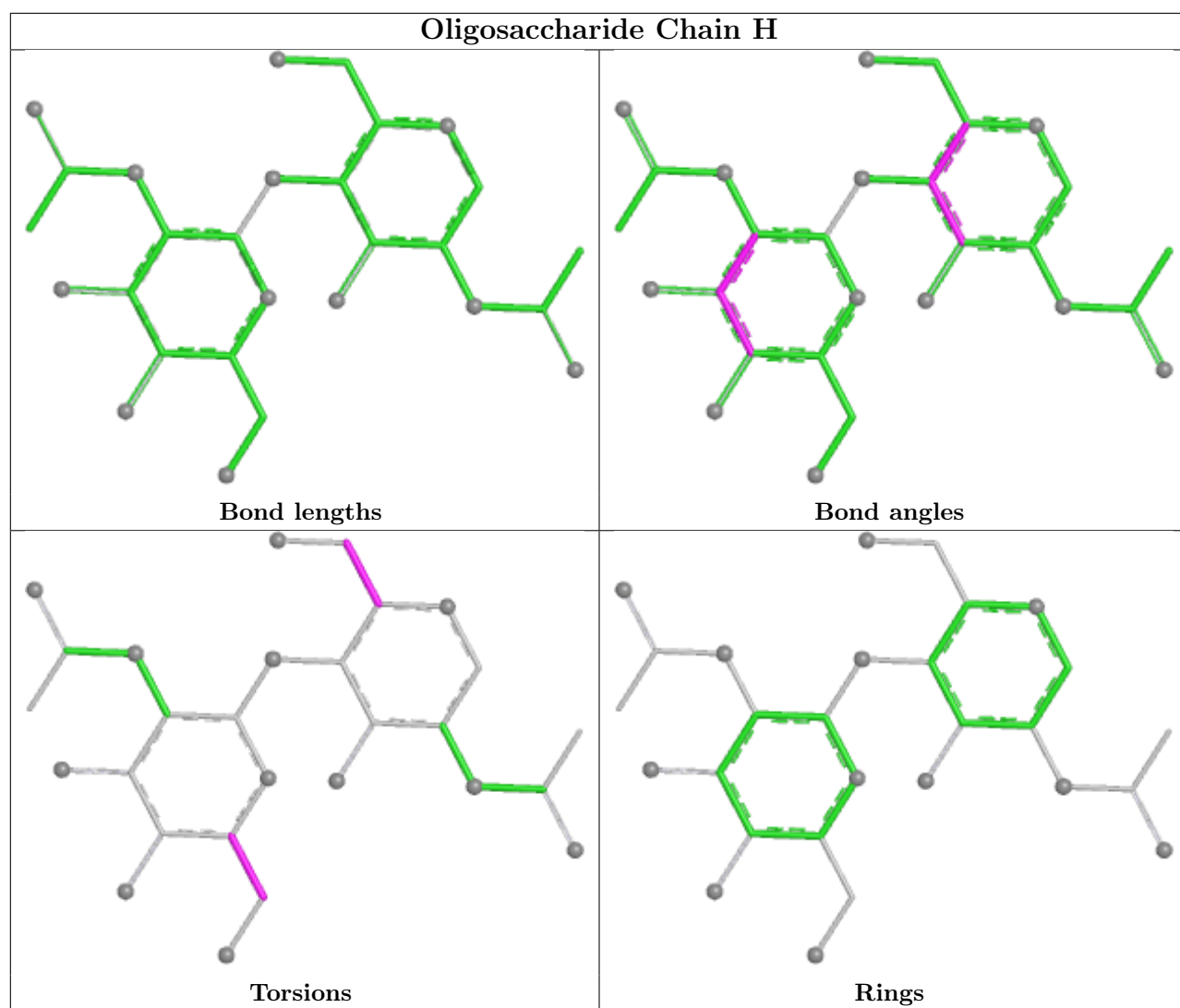
Mol	Chain	Res	Type	Atoms
7	M	1	NAG	O5-C5-C6-O6
8	I	5	MAN	O5-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
8	I	6	MAN	O5-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
8	I	3	BMA	C4-C5-C6-O6
7	J	2	NAG	C4-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
7	M	2	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
9	N	1	NAG	C1-C2-N2-C7
9	N	3	BMA	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
9	N	1	NAG	C3-C2-N2-C7
7	K	1	NAG	C4-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6

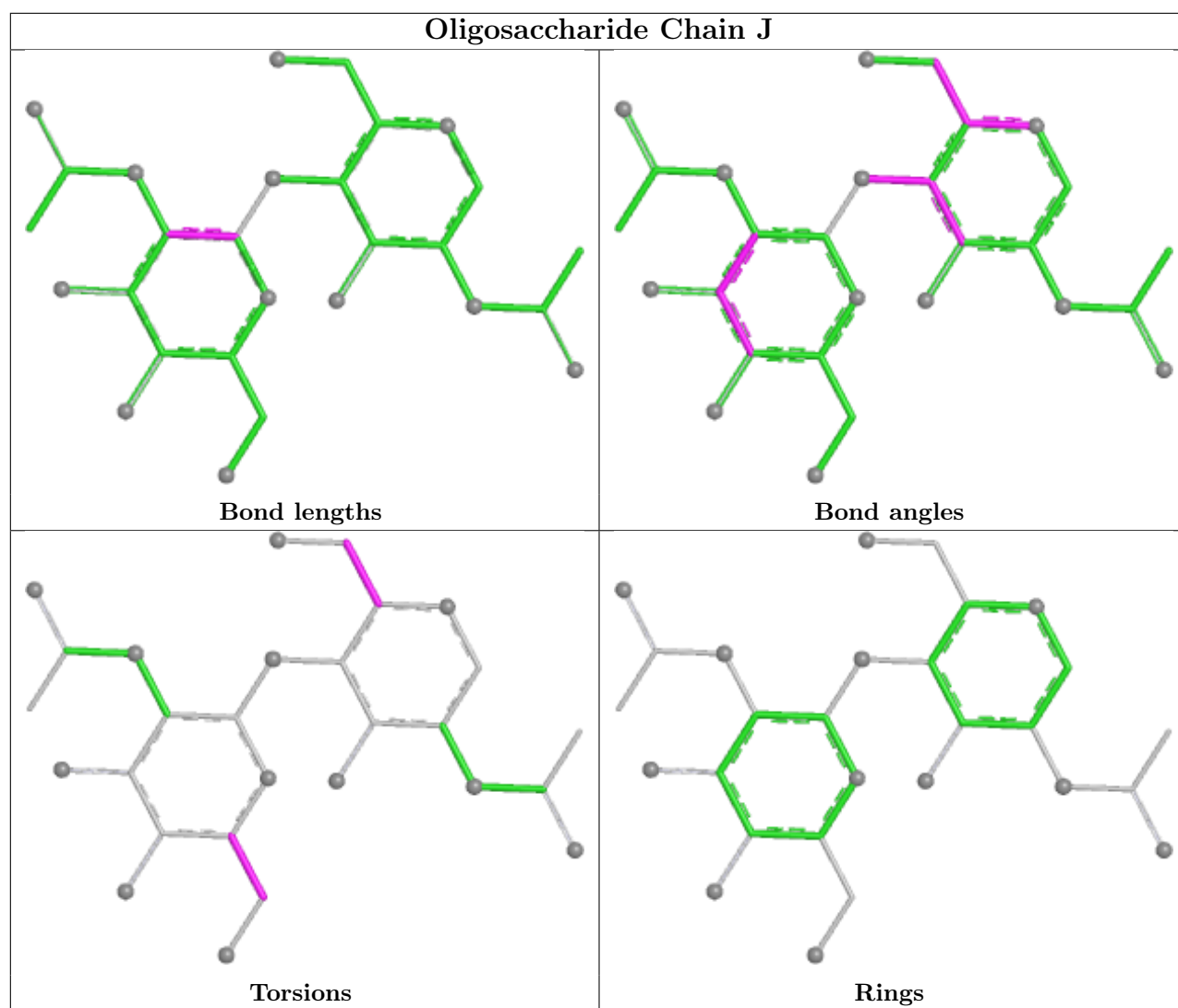
There are no ring outliers.

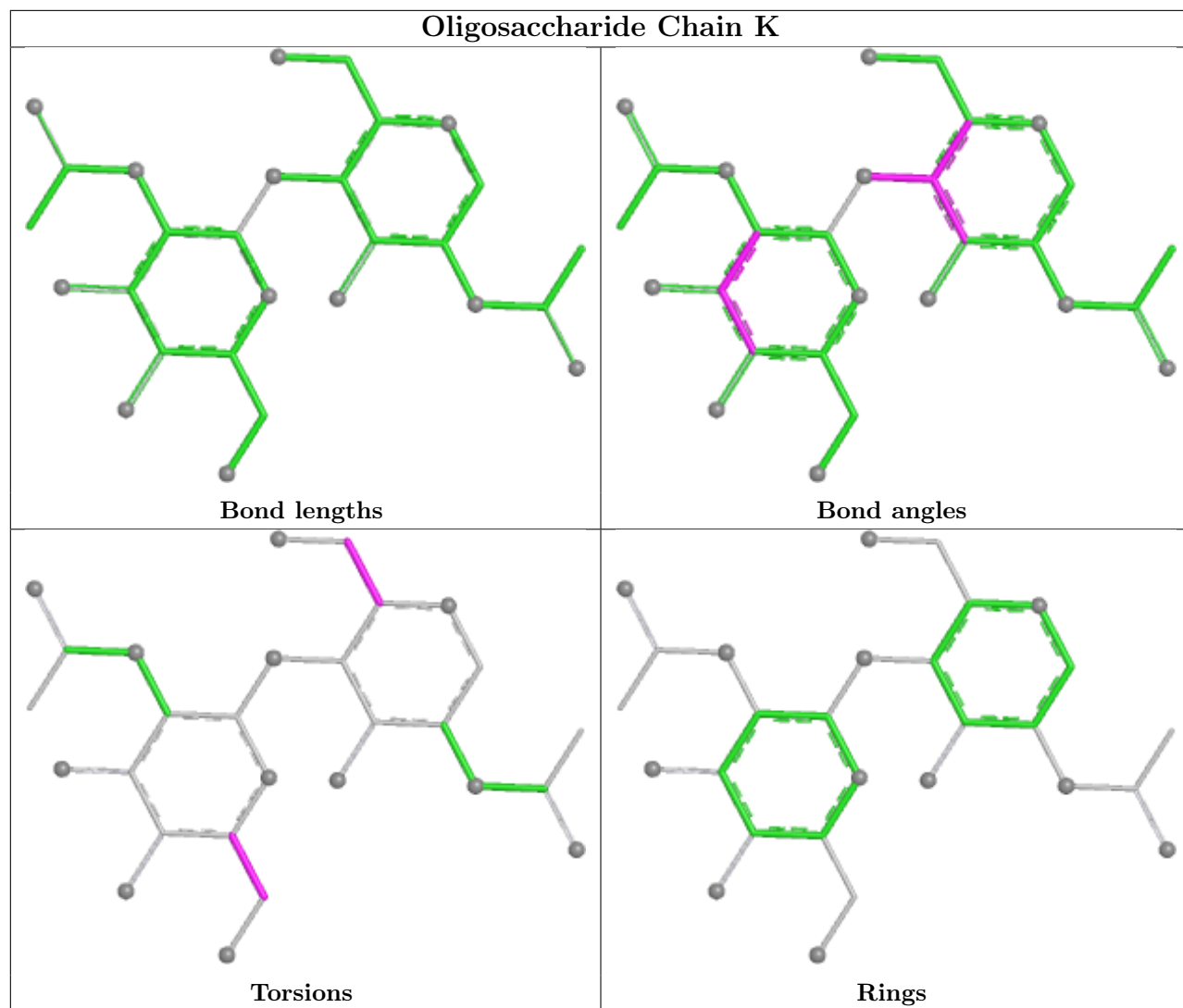
No monomer is involved in short contacts.

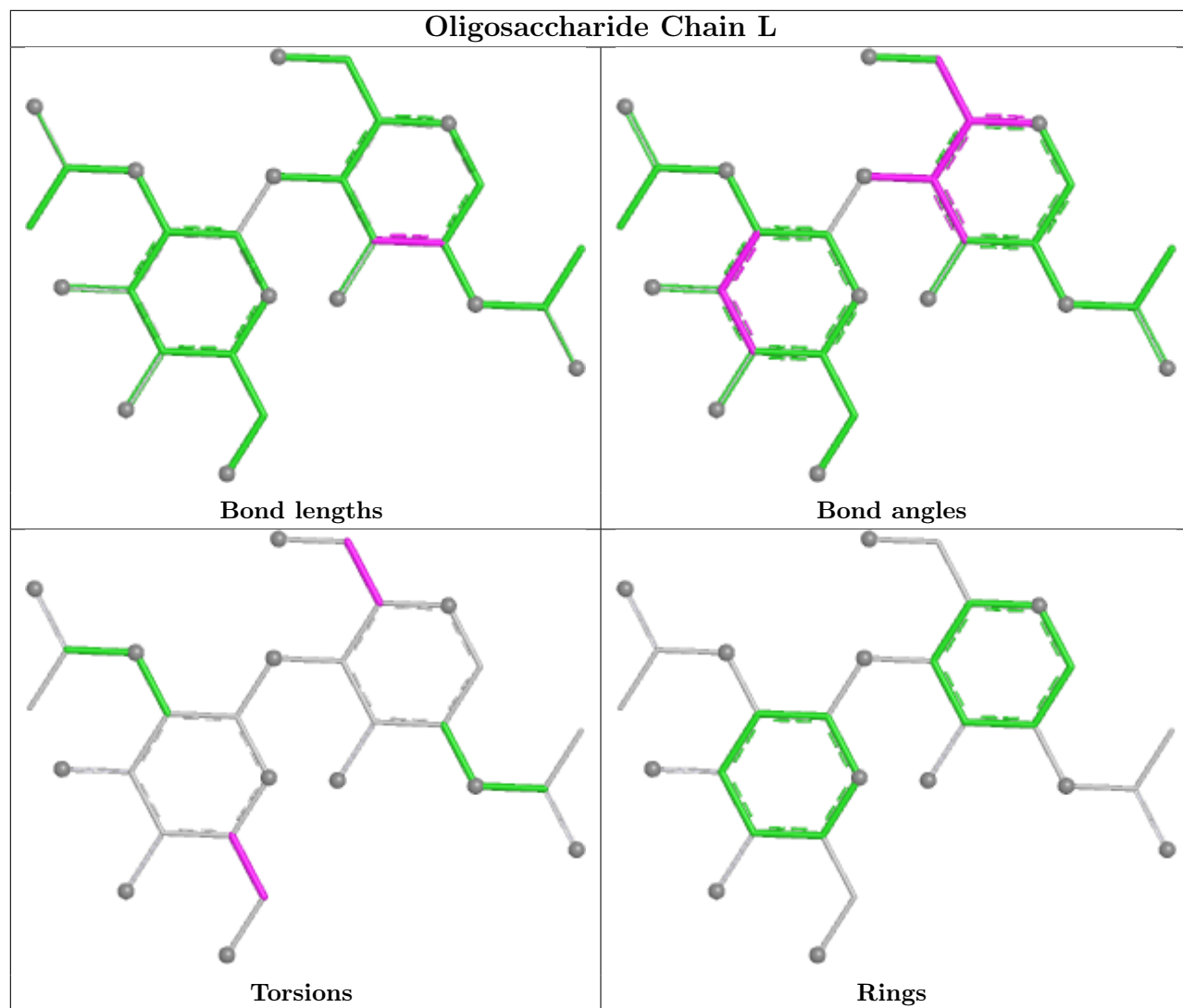
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

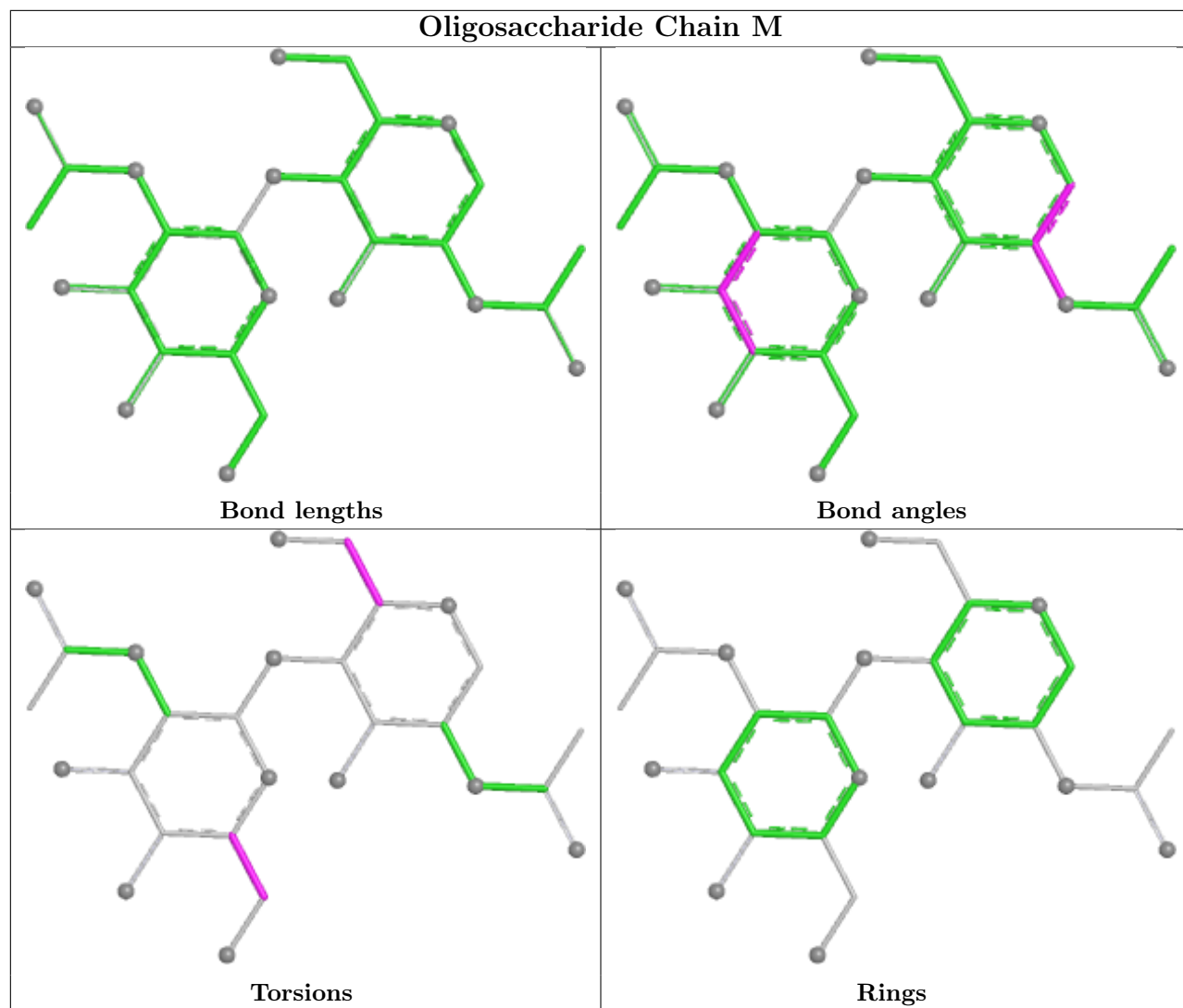


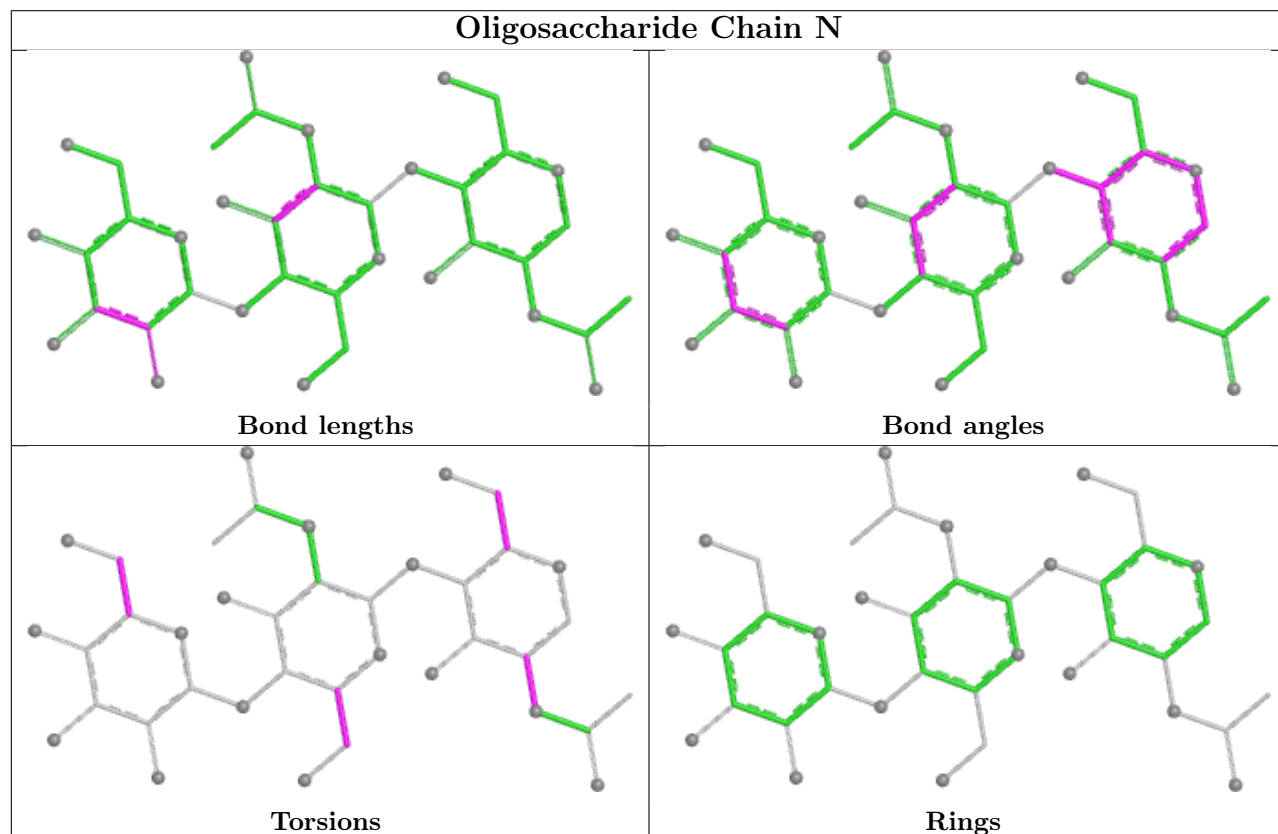
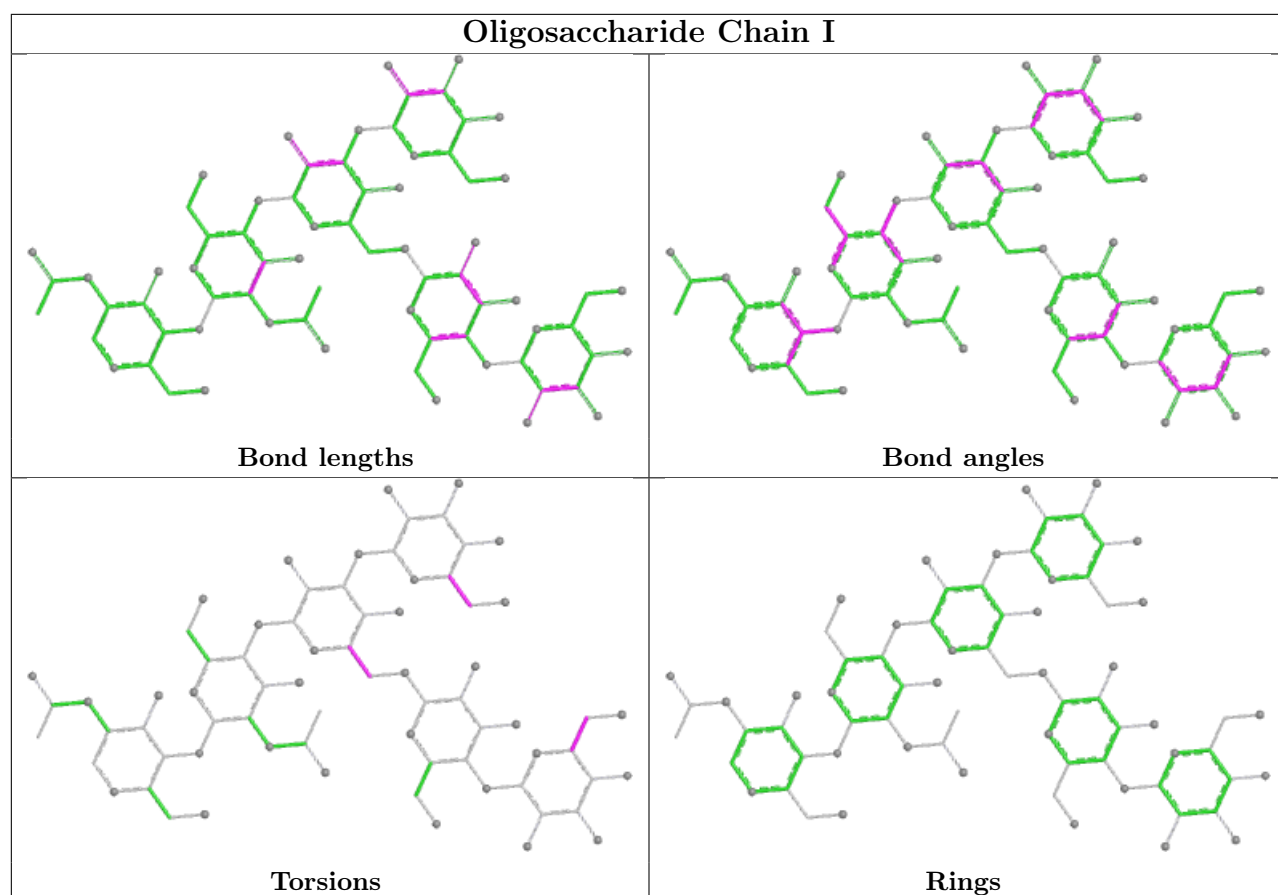












5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	B	701	2	14,14,15	0.88	0	17,19,21	0.99	1 (5%)
10	NAG	A	1011	1	14,14,15	0.80	0	17,19,21	0.92	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	701	2	-	1/6/23/26	0/1/1/1
10	NAG	A	1011	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	701	NAG	C4-C3-C2	-2.94	106.71	111.02
10	A	1011	NAG	C4-C3-C2	-2.74	107.00	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1011	NAG	O5-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

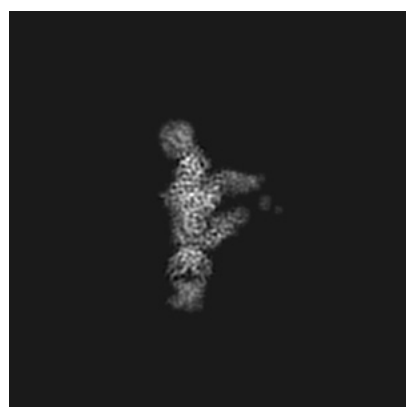
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7939. These allow visual inspection of the internal detail of the map and identification of artifacts.

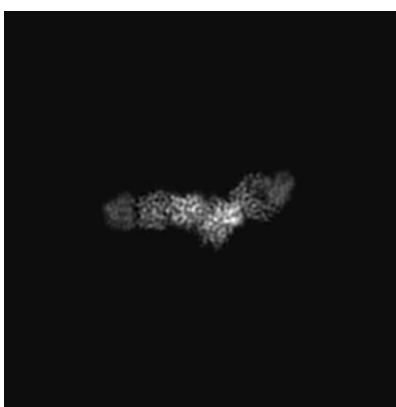
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

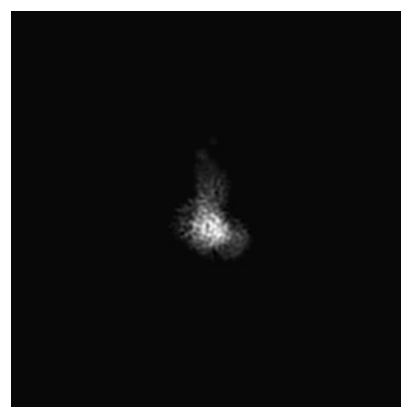
6.1.1 Primary map



X



Y

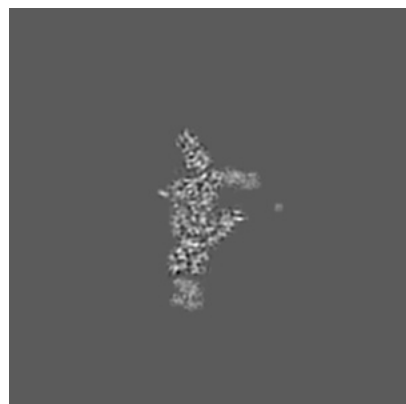


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

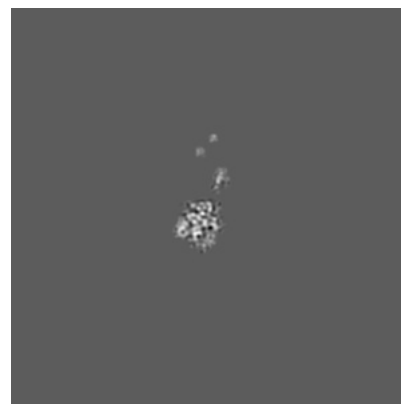
6.2.1 Primary map



X Index: 128



Y Index: 128

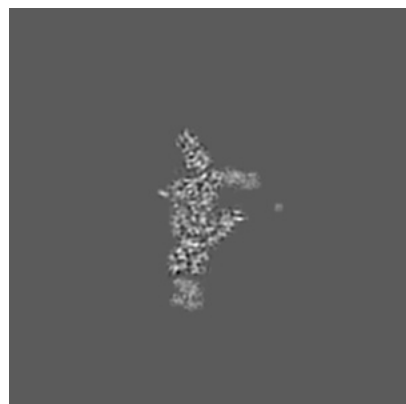


Z Index: 128

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 128



Y Index: 115

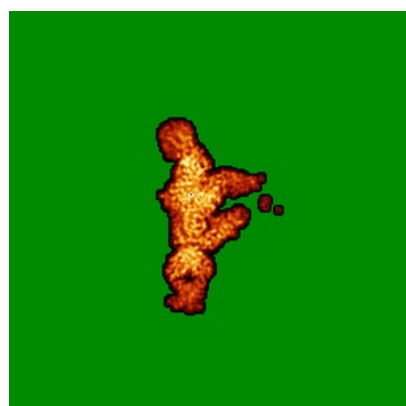


Z Index: 137

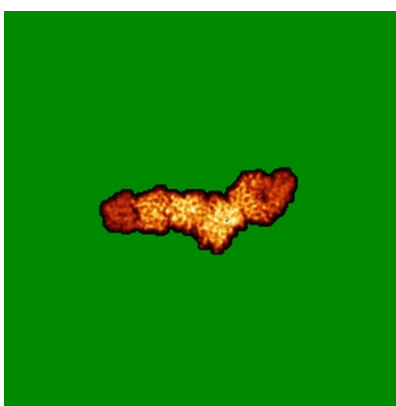
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

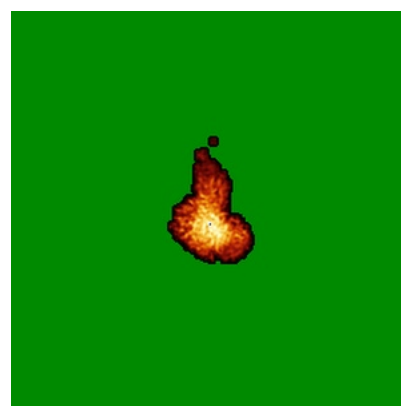
6.4.1 Primary map



X



Y

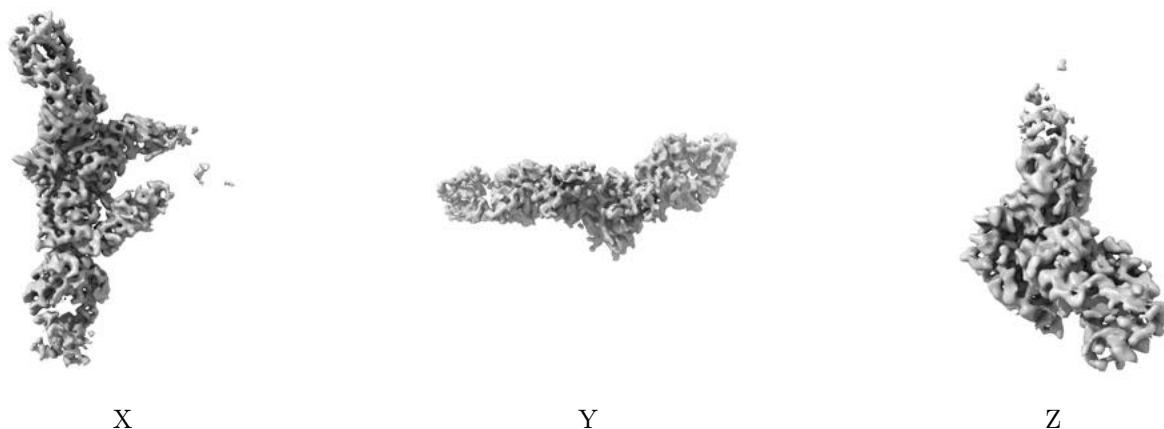


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

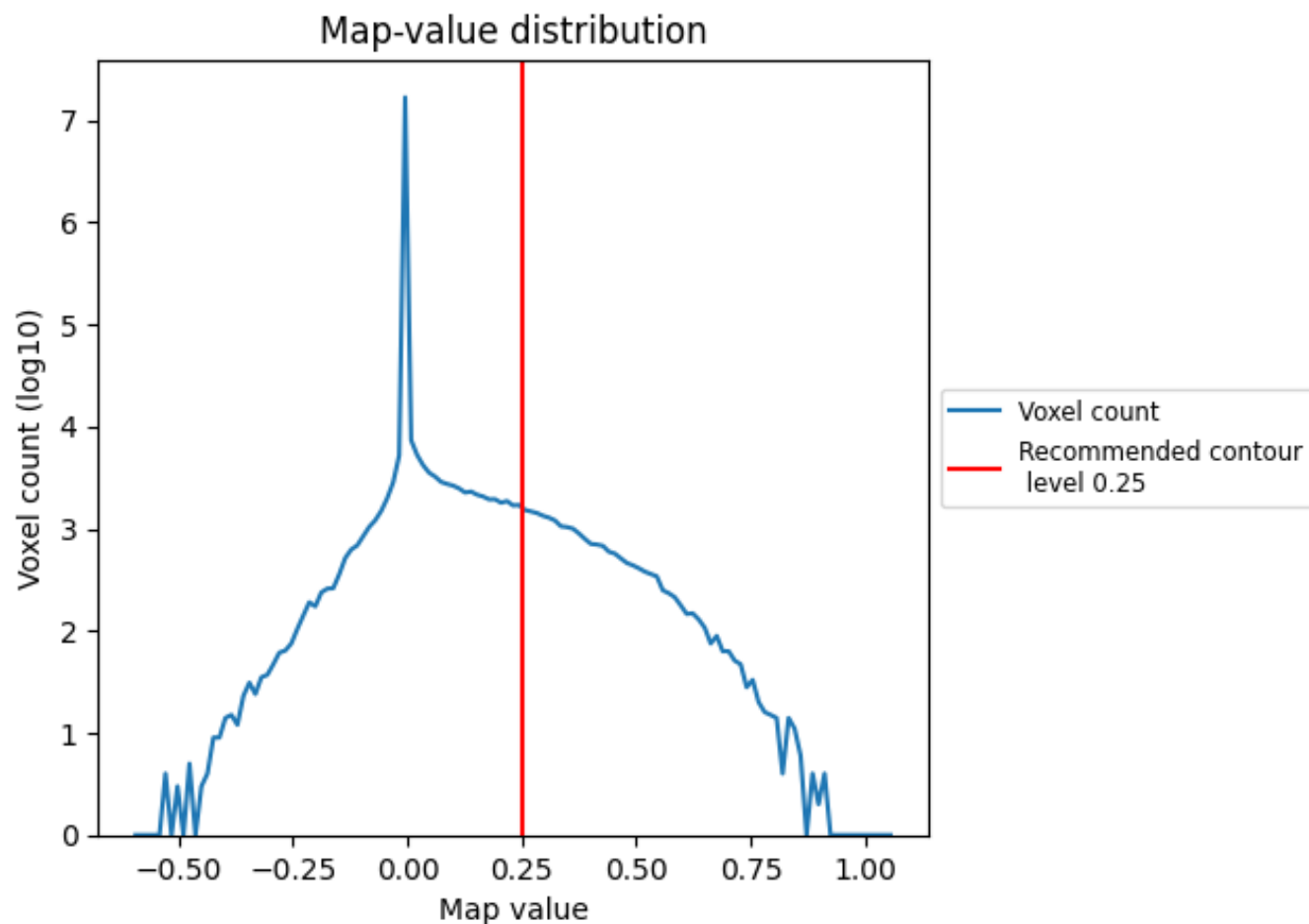
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

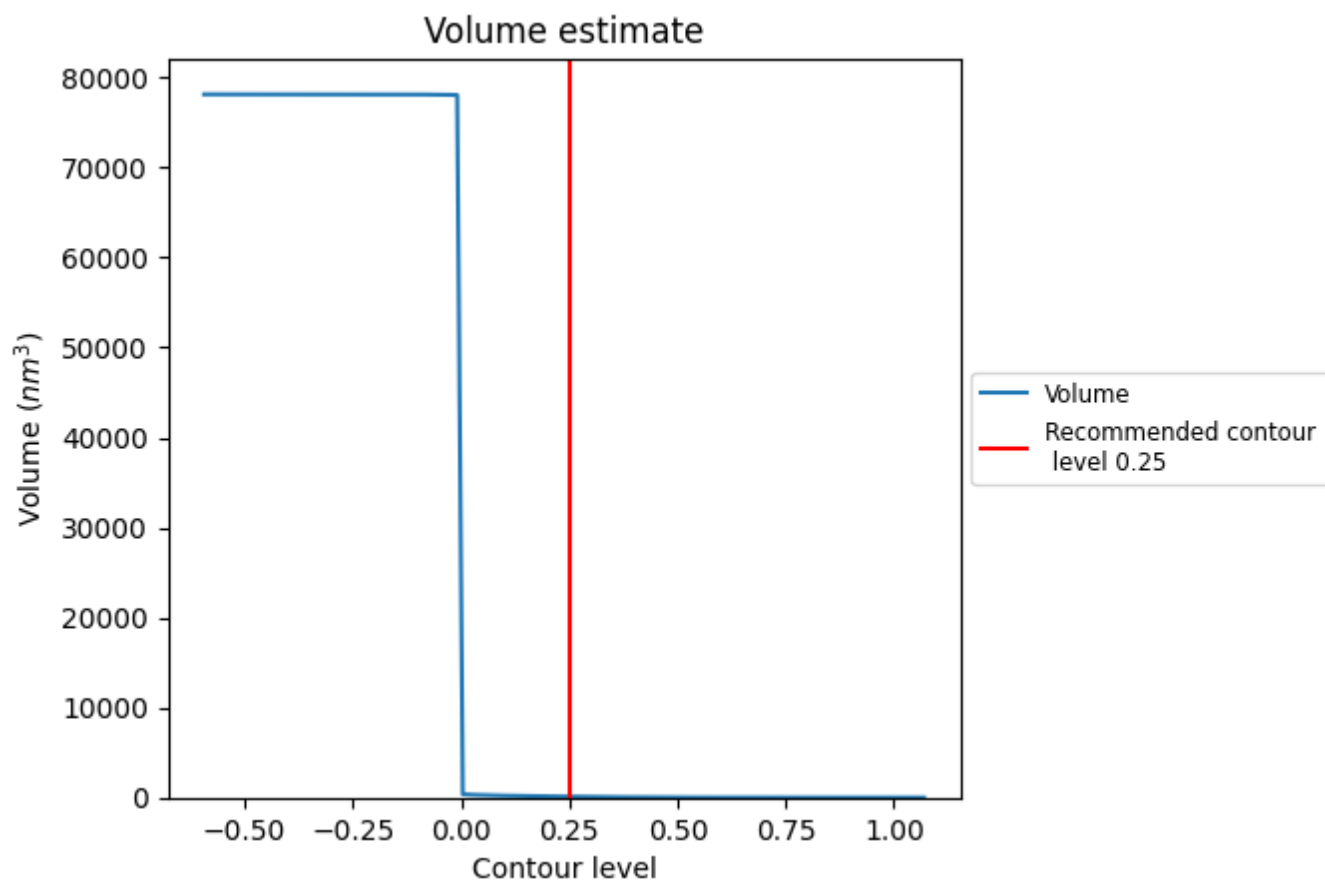
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

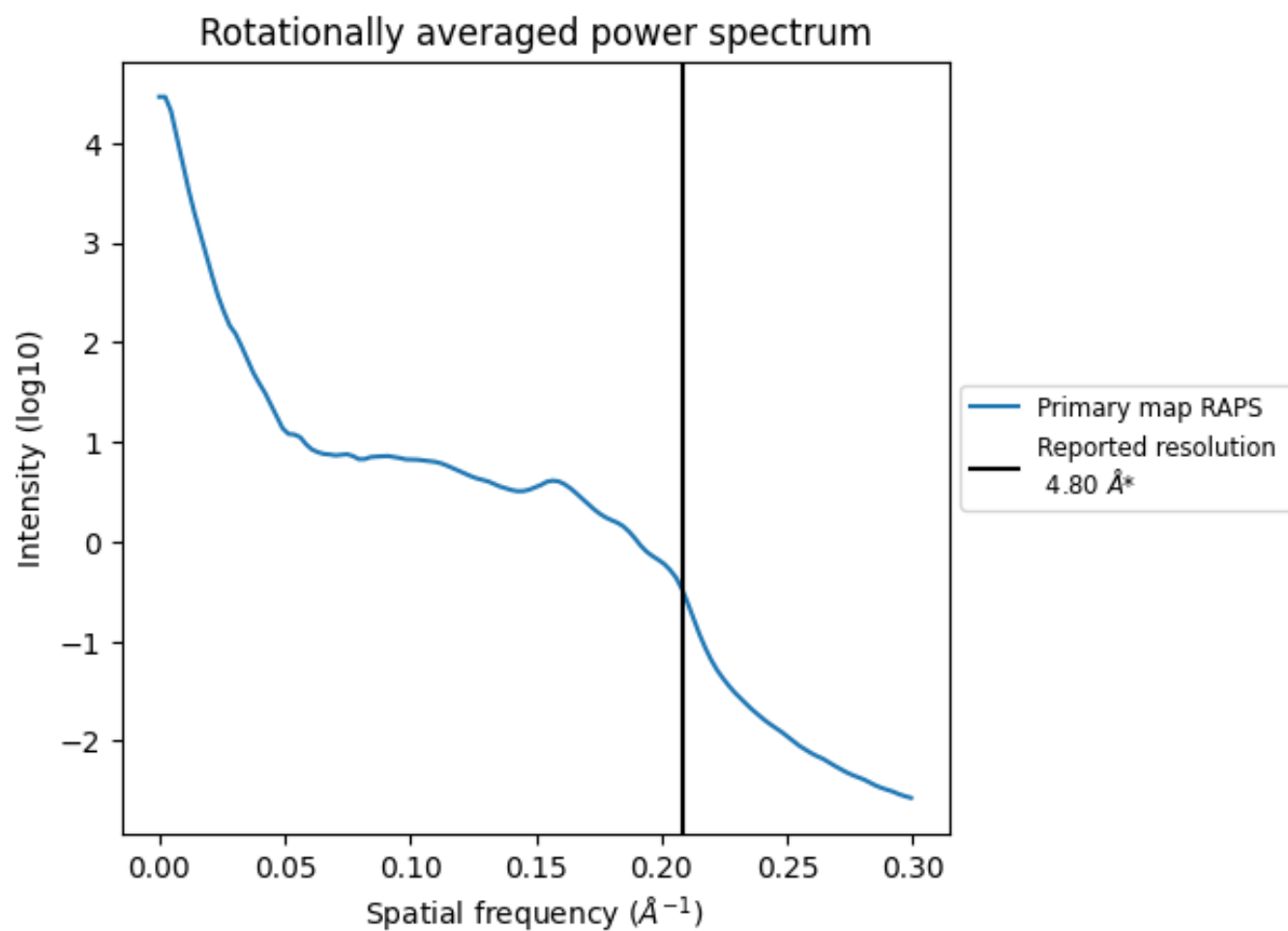
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

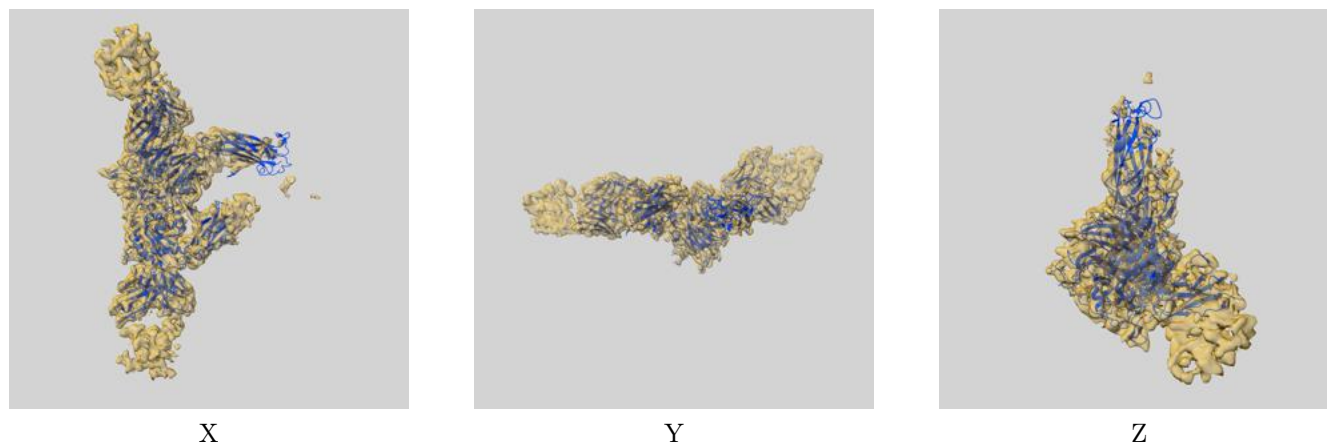
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

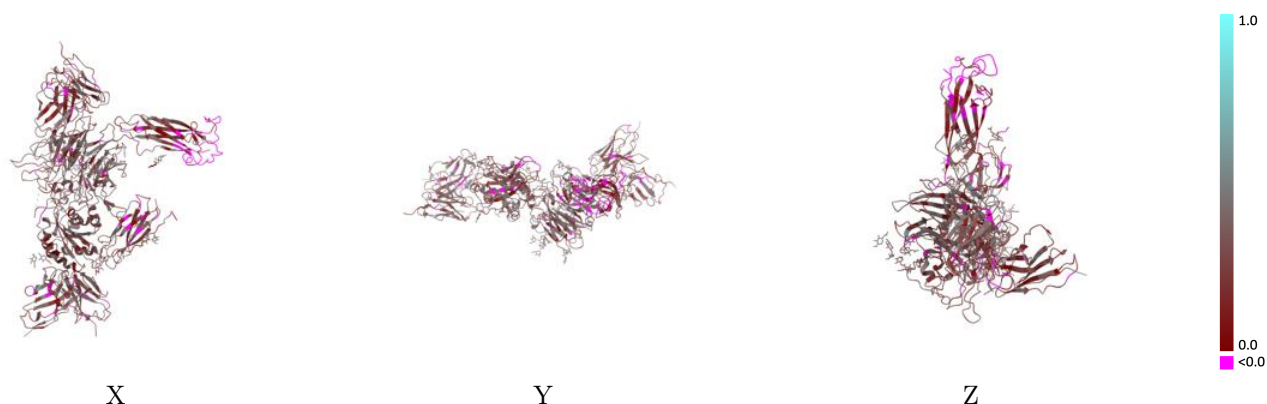
This section contains information regarding the fit between EMDB map EMD-7939 and PDB model 6DJP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



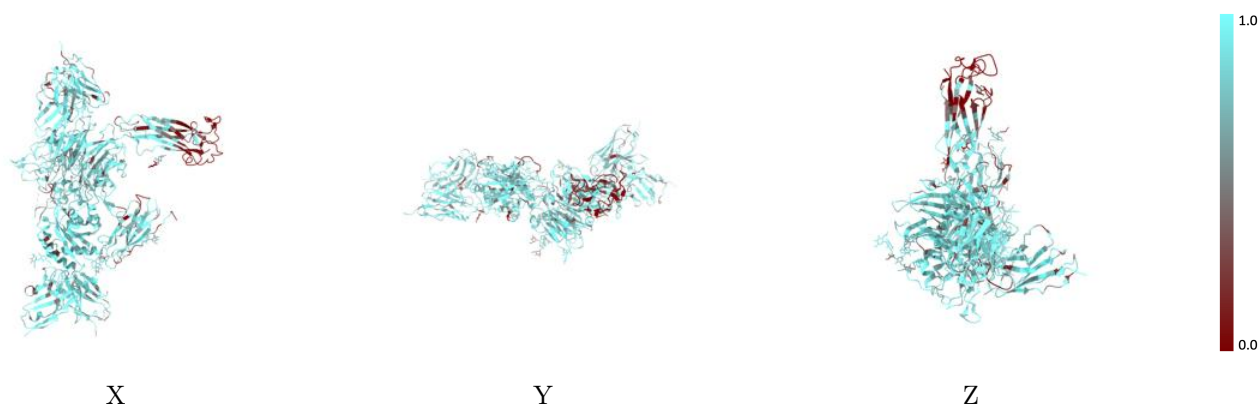
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



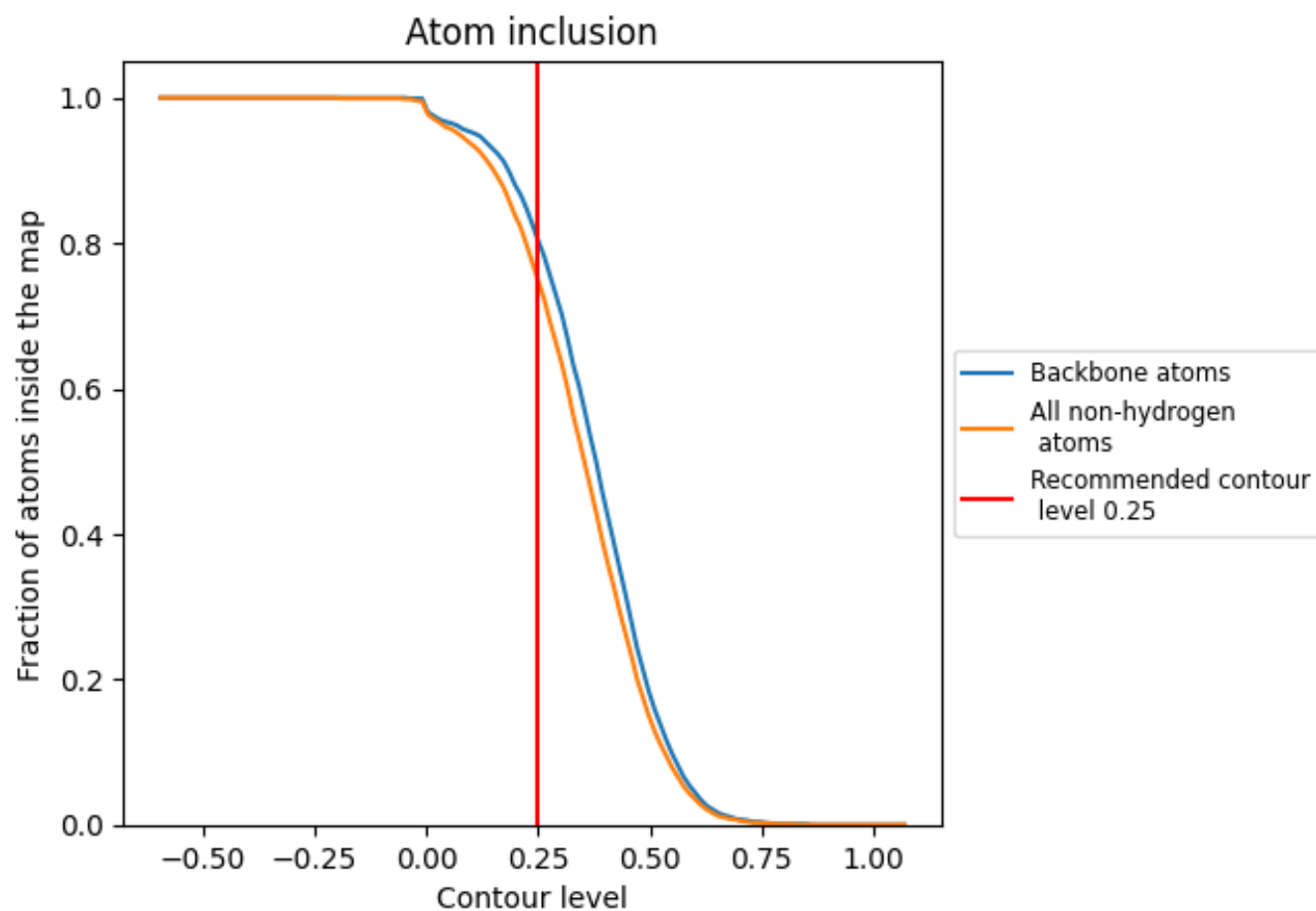
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.2750
A	 0.7110	 0.2590
B	 0.7870	 0.2910
C	 0.7590	 0.2480
D	 0.7650	 0.2700
E	 0.7890	 0.2750
F	 0.8300	 0.3040
G	 0.6430	 0.3400
H	 0.8570	 0.3850
I	 0.6390	 0.3470
J	 0.3210	 0.2710
K	 0.7860	 0.4170
L	 0.3930	 0.4160
M	 0.7140	 0.3340
N	 0.6920	 0.3320

